OUTLINE

Melt Spun Fibers Or Other Forms For Selective Filtration of Tobacco Smoke

- POTENTIAL OF POLYMERS FOR SELECTIVE FILTRATION
- STRATEGIC ELEMENTS OF THE PROGRAM
- THE SELECTIVE FILTRATION TEST APPARATUS
- THE SELECTIVE FILTRATION TEST PROCEDURES
- CURRENT DATA HANDLING STRATEGY
- STATUS OF PROGRAM -- DECEMBER 1993
- APPROACH TO SOLVE THE CURRENT PROBLEM
- REVISED MILESTONES

EXPECTED POLYMER/CHEMICAL INTERACTIONS

POTENTIAL OF POLYMERS FOR SELECTIVE FILTRATION

A CHEMICAL WILL DISSOLVE IN A POLYMER IF THE GIBBS FREE ENERGY OF THE PROCESS IS NEGATIVE.

$$\Delta F = \Delta H - T\Delta S$$

ΔF Change in Gibbs Free Energy in a Process
ΔH Change in Enthalpy in a Process
T Absolute Temperature of a Process
ΔS Change in Entropy of a Process

FOR A SOLUTION, ΔS WILL BE POSITIVE SINCE THE MOLECULES OF A SOLUTION ARE MORE RANDOMIZED THAN IN NEAT STATES.

$-T\Delta S$ WILL BE NEGATIVE WHICH FAVORS SOLUBILITY

ΔH CAN BE POSITIVE OR NEGATIVE

$+\Delta H$ INDICATES SEPARATE COMPONENTS ARE LOWER ENERGY

$-\Delta H$ INDICATES MIXTURE HAS A LOWER ENERGY STATE

A NEGATIVE ΔH OCCURS WITH **SPECIFIC INTERACTIONS** WHICH **ASSURES SOLUTION OF A CHEMICAL IN A POLYMER**

WITHOUT SPECIFIC INTERACTIONS, ΔH IS POSITIVE. SINCE $T\Delta S$ IS SMALL FOR POLYMERS, **SOLUBILITY OCCURS** WHEN $\Delta H \rightarrow$ ZERO, WHICH OCCURS **WHEN SOLUBILITY PARAMETERS FOR THE CHEMICAL AND THE POLYMER APPROACH EACH OTHER.**

$$\Delta H \approx \Delta E = \phi_1\phi_2(\delta_1 - \delta_2)$$

ΔE = Change in Internal Energy
ϕ = Volume Fractions
δ = Solubility Parameters

$$= (CED)^{1/2} = (\Delta E_v/v)^{1/2}$$

(CED) = Cohesive Energy Density, a measure of intermolecular forces (measured from heats of vaporization)
ΔE_v = Molar change in internal energy on vaporization
v = Molar volume of liquid

2023957003

CROWLEY, TEAGE & LOWE
JOURNAL OF PAINT TECHNOLOGY, 38, #496 MAY 1966 p 273

Table 4 (cont'd)—Listing of Solvents by Increasing δ

Solvent	Solubility Parameter, δ	Hydrogen Bonding, γ	Dipole Moment, μ
Chloroform	9.3	1.5	1.2
Methyl ethyl ketone	9.3	7.7	2.7
Methyl propionate	9.3	8.4	1.9
Styrene (monomer)	9.3	1.5	0
n-Butyl lactate	9.4	7.0	1.9
Capronitrile	9.4	7.7	4.0
Ethyl formate	9.4	8.4	1.9
Chlorobenzene	9.5	1.5	1.6
Ethyl hexanol (2)	9.5	18.7	1.7
Diethylene glycol monoethyl ether	9.6	13.0	1.6
Methyl acetate	9.6	8.4	1.7
Trichloroethane (1,1,2)	9.6	1.5	1.2
Cyclohexanone	9.7	11.7	2.7
Methylene chloride	9.7	1.5	1.5
Ethylene dichloride	9.8	1.5	1.1
Anisole	9.9	7.0	1.4
Ethylene glycol monoethyl ether	9.9	13.0	1.6
Diethylacetamide (N,N)	9.9	12.3	2.0
Dimethyl carbonate	9.9	4.9	1.0
Dioxane (1,4)	9.9	9.7	0
Acetone	10.0	9.7	2.9
Carbon disulfide	10.0	0	0
Ethyl lactate	10.0	7.0	1.9
Methyl isobutyl carbinol	10.0	18.7	1.7
Nitrobenzene	10.0	2.8	4.3
Methyl formate	10.2	8.4	1.9
Octyl alcohol	10.3	18.7	1.7
Cyclopentanone	10.4	8.4	2.7
Methyl benzoate	10.4	6.3	1.9
Phenyl acetate	10.4	7.7	1.9
Acrylonitrile	10.5	5.7	3.8
Butyronitrile	10.5	7.7	4.0
Diethylformamide (N,N)	10.6	11.7	2.0
n-Hexyl alcohol	10.7	18.7	1.7
Nitropropane	10.7	2.5	3.7
Pyridine	10.7	18.1	2.2
Acetyl acetone	10.8	8.4	3.1
Dimethylacetamide (N,N)	10.8	12.3	2.0
Propionitrile	10.8	7.7	4.0
Ethylene oxide	11.1	10.0	1.9
Nitroethane	11.1	2.5	3.6
Dipropyl sulfone	11.3	7.7	4.5
n-Butyl alcohol	11.4	18.7	1.7
Cyclohexanol	11.4	18.7	1.7
Aniline	11.8	18.1	1.5
Acetonitrile	11.9	6.3	3.9

between the solubility parameters of a liquid and a not too polar amorphous polymer can be related to the heat change in their mixing and the interaction of polymer and liquid will therefore depend, in part, on the solubility parameter of the latter.

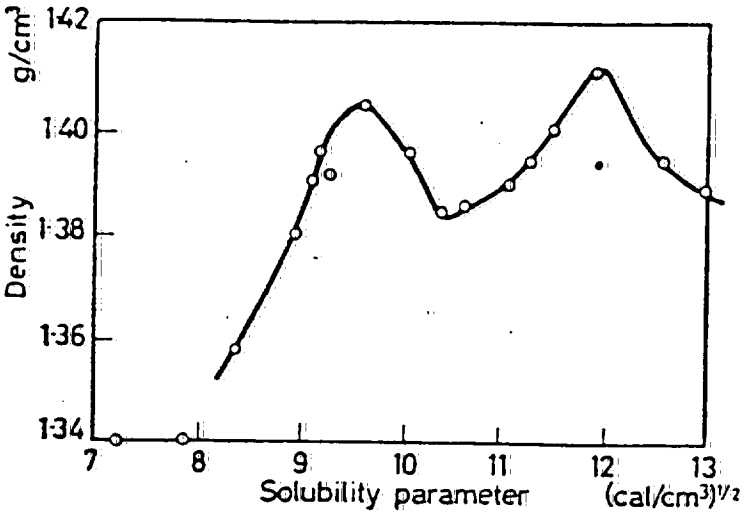


Figure 2 — Equilibrium density as a function of solubility parameter of liquid

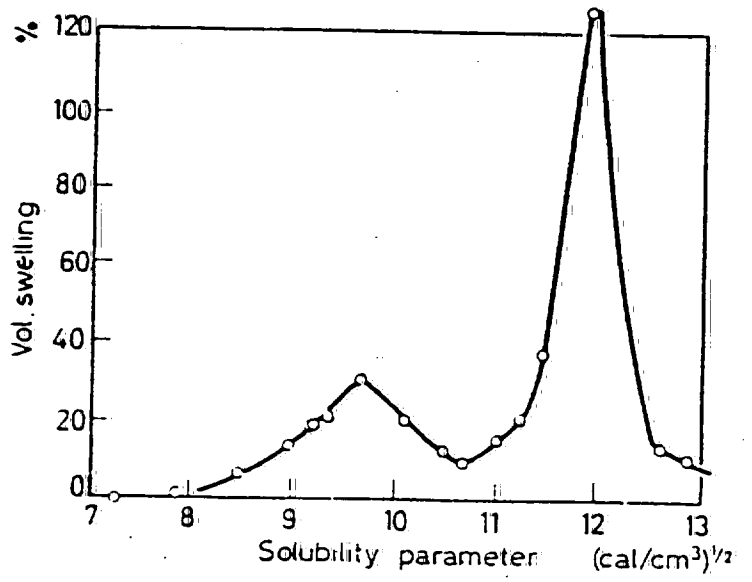


Figure 3—Equilibrium swelling as a function of solubility parameter of liquid

Figure 2 shows two maxima at δ values of approximately 9·7 and 12·0 and similar maxima are seen in *Figure 3*. The first maximum is associated with liquids such as ketones and esters which may be regarded as basic in the Lewis sense. Benzene and toluene, which are associated with this region of the plots, can also be regarded as basic[11]. The second maximum is associated with liquids of acidic type such as *m*-cresol, acetic acid and nitromethane. The existence of two maxima may be a consequence of the presence of basic carbonyl groups in the polymer and acidic hydrogen atoms in CH groups adjacent to oxygen atoms. Gilbs *et al*[12] have suggested that

molar energies or enthalpies of vaporization as noted above. High polymers, the other hand, cannot be vaporized (because of their size they have enormous cohesive energies) without decomposition; their solubility parameters must be determined indirectly. Several methods have been employed, most of which use a series of potential solvents with known solubility parameters. In one method the solubility parameter δ_2 for the macromolecule is taken as the midpoint of the range of δ_1s for those liquids that completely dissolve the polymer. If the polymer is not completely miscible, δ_2 is equated to the solubility parameter δ_1 of the liquid in which it has the greatest solubility. In another method the swelling of a lightly cross-linked polymer is measured in the various liquids. The greatest swellings should be found with solvents for which $\delta_1 \approx \delta_2$. The variation of the intrinsic viscosity of the polymer solution with the solubility parameter of the solvent provides yet another method for evaluating δ_2. The viscosity is greatest when $\delta_1 \approx \delta_2$. It is also possible to estimate solubility parameters by summing group contributions (29–31). These and other procedures have been summarized (32). Solubility parameters for large numbers of polymers and solvents have been compiled (30,33).

The solubilities of four polymers in 13 solvents that cover a wide range of solubility parameters have been tabulated (34). This analysis, shown here as Table 2, demonstrates the practical utility of the solubility-parameter method.

SOLUBILITY OF POLYMERS
ENCYCLOPEDIA of POLYMER SCIENCE & ENGINEERING 2nd ed V15 p 394

Table 2. Solubilities[a] and Solubility Parameters[b] of Polymer–Solvent Systems[c]

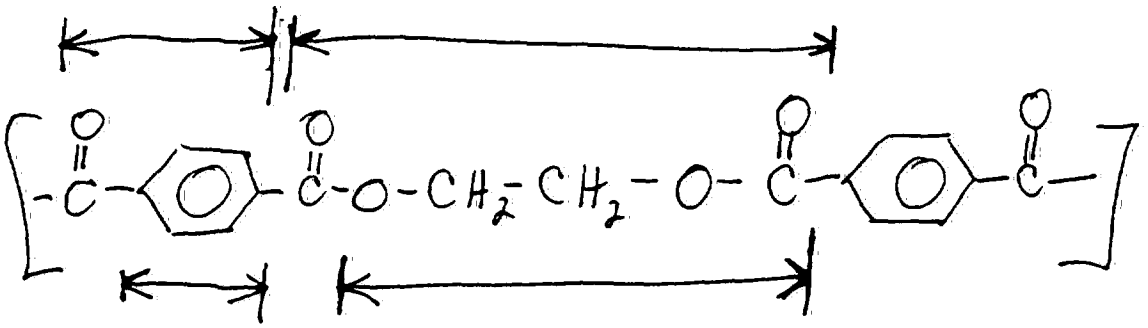
Name	δ_1	Polyisobutylene (δ_2 = 16.2)	Poly(methyl methacrylate) (δ_2 = 18.6)	Poly(vinyl acetate) (δ_2 = 19.2)	Poly(hexamethylene adipamide) (δ_2 = 27.8)
decafluorobutane	10.6	–	–	–	–
neopentane	12.9	+	–	–	–
n-hexane	14.9	+	–	–	–
diethyl ether	15.1	–	–	–	–
cyclohexane	16.8	+	–	–	–
carbon tetrachloride	17.6	+	+	–	–
benzene	18.8	+	+	–	–
chloroform	19.0	+	+	+	–
methyl ethyl ketone	19.0	–	+	+	–
acetone	20.3	–	+	+	–
carbon disulfide	20.5	–	–	–	–
1,4-dioxane	20.5	–	+	+	–
dimethylformamide	24.8	–	+	+	(+)
m-cresol	27.2	–	+	+	+
formic acid	27.6	–	+	–	–
methanol	29.7	–	–	–	–
water	47.9	–	–	–	–

[a] + soluble, – insoluble, (+) soluble at high temperatures only.

[b] The solubility parameters in this table have units of $(J/cm^3)^{1/2}$. To convert to $(cal/cm^3)^{1/2}$, divide by 2.05.

[c] Ref. 34. Courtesy of Plenum Publishing Corp., 1984.

20239706



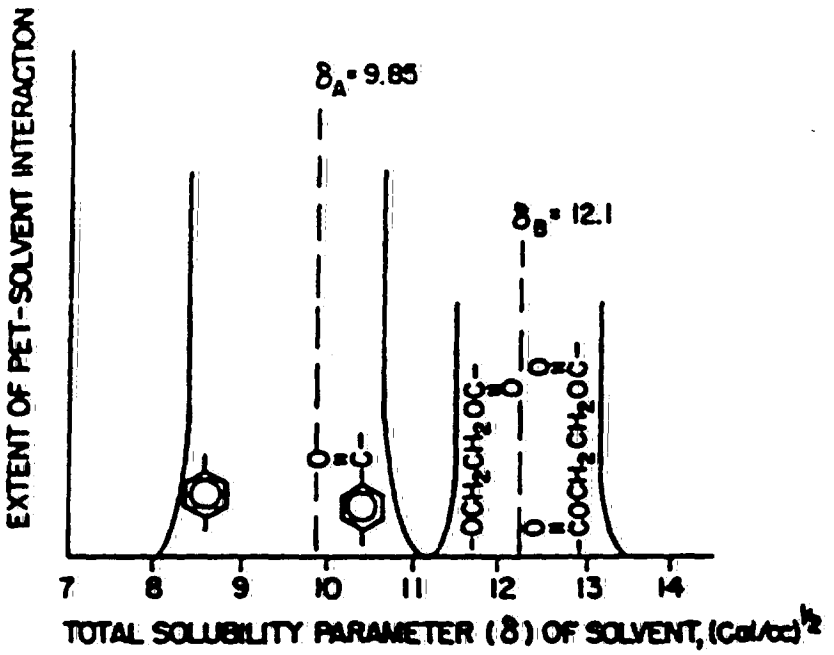


Fig. 9. Schematic representation of the anomalous broadening of the Hildebrand solubility p rameter distribution curve associated with the aromatic residue A in which the chemical structur comprising the "hybrid" structures are positioned on the bimodal plot at their respective total s ubility parameters (δ).

B. H. KNOX
J. APPL. POLY. SCI., 21, 249-266 (1977)

KNOX, WEIGMANN & SCOTT

TEXTILE RESEARCH JOURNAL
MARCH 1975 p 208

age and crystallinity of polyester yarn
ingle solvent treatment at 40°C.

ge Shrinkage (single), %	Density (single), g/cm³	Crystallinity (single), %
—	1.3770	35.0
7.4	1.3797	37.2
8.4	1.3812	38.5
10.2	1.3815	38.8
11.4	1.3832	40.2
20.0	1.4027	56.4

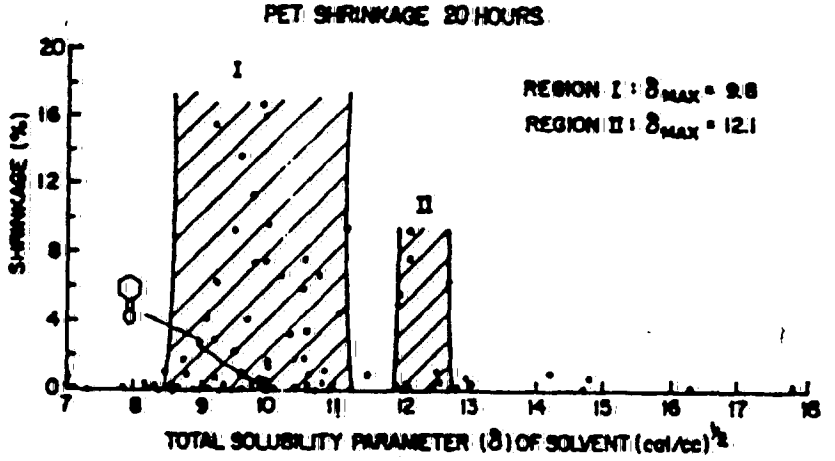


FIG. 1. Solvent-induced shrinkage of drawn PET after 20 h at 21°C *versus* total solubility parameter δ of solvent.

calculated from density data for
atment using the formula:

$$\text{nity } (\%) = \frac{d_{exp.} - d_a}{d_c - d_a},$$

he amorphous polyester $d_a = 1.335$
stalline density $d_c = 1.455$ g/cm³

t column was prepared with a mix-
nd carbon tetrachloride according
5 test procedure. Calibrated floats
om 1.54 to 1.44 g/cc were used.
yarns were de-aerated in the same
placed in the column, and their
column were read with a cathe-
2 h at 23 ± 0.2°C.

Results

RINKAGE. The degree of longi-
conveniently defined in terms of

be expected to cause high levels of longitudinal shrinkage; yet after a period of 20 h, and even after a period of 3 months, only low levels of shrinkage are developed. This appears to indicate that the total solubility parameter does not adequately describe the observed experimental behavior.

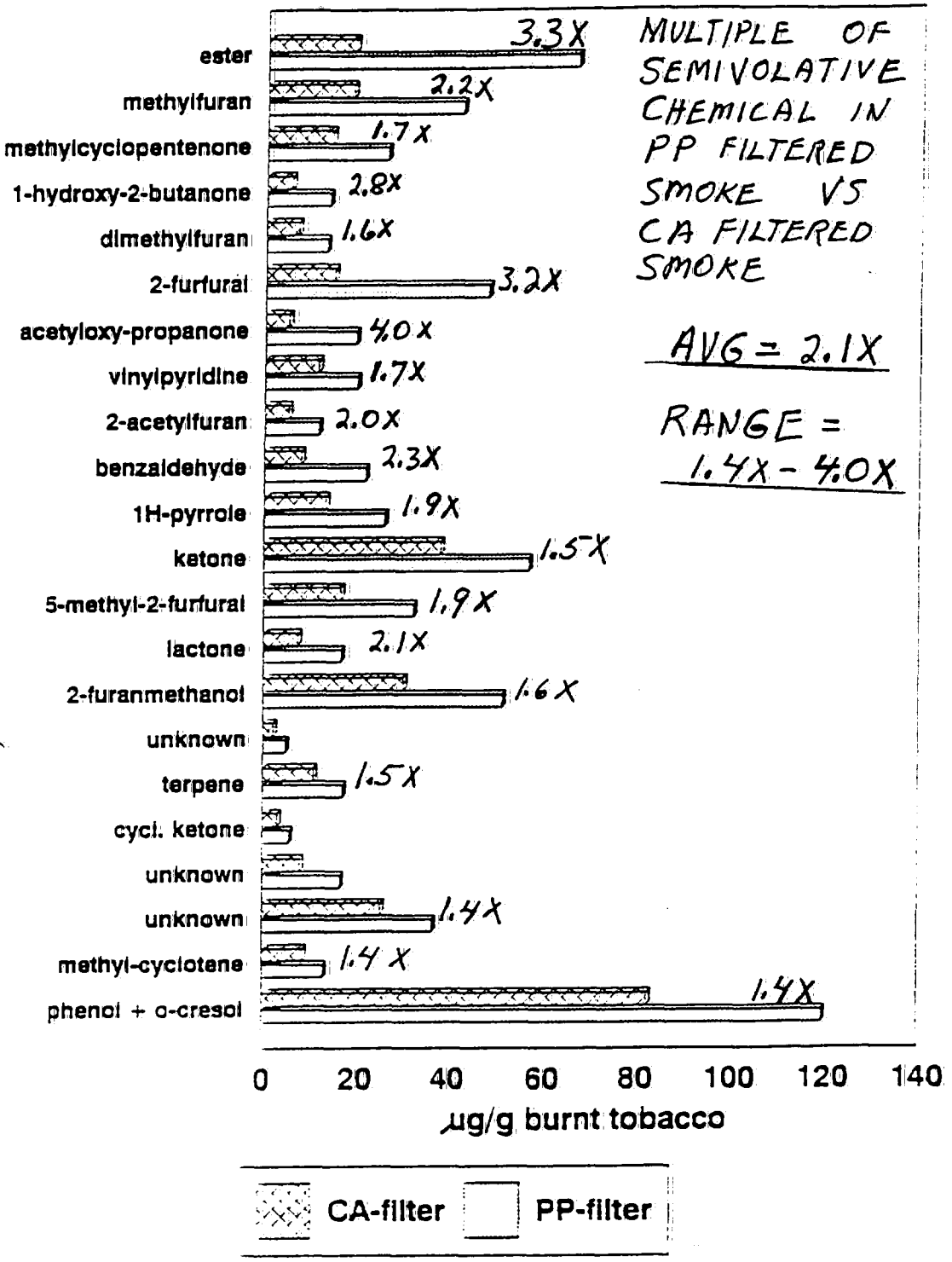
It is apparent from the brief theoretical discussion of the solubility parameter concept, that it would be more meaningful to express the shrinkage data in Figure 1 by a Hansen two-dimensional solubility parameter plot. If shrinkage is so represented (see Fig. 2), it can be shown that cyclohexanone actually falls outside both areas of high PET-solvent interaction, and that cyclohexanone would therefore be expected to interact only slightly with PET, as observed experimentally. The choice of three percent shrinkage as a cutoff point in classifying a given liquid either as a "non-solvent" or as a "solvent" is arbitrary and was made to show the existence of two areas of PET-solvent interactions and to maximize the percent correlation (to be defined later).

Table 1
APPROXIMATE HILDEBRAND PARAMETER (δ) RANGES FOR SOME COMMON POLYMERIC MATERIALS, CLASSIFIED BY HYDROGEN BONDING CAPABILITY AND IN ORDER OF INCREASING δ VALUES[1362,1363]

Polymer	Hildebrand parameter ranges (δ/MPa$^{1/2}$) in solvents with hydrogen bonding capability which is		
	Poor	Moderate	Strong
Polytetrafluorocarbons	12—13	—	—
Ester gum	14—22	15—22	19—22
Alkyd 45% soy oil	14—22	15—22	19—24
Silicone DC-1107	14—19	19—22	19—24
Poly(vinyl ethyl ether)	14—23	15—22	19—29
Poly(butyl acrylate)	14—26	15—24	—
Poly(butyl methacrylate)	15—23	15—20	19—23
Silicone DC-23	15—17	15—16	19—21
Polyisobutylene → SIMILAR TO PP	15—16	—	—
Polyethylene	16—17	—	—
Gilsonite®	16—19	16—17	—
Poly(vinyl butyl ether)	16—22	15—21	19—23
Natural rubber	17	—	—
Hypalon® 20 [chlorosulfonated PE]	17—20	17—18	—
Ethyl cellulose N-22	16—23	15—22	19—30
Chlorinated rubber	17—22	16—22	—
Dammar gum	17—22	16—21	19—22
Versamid® 100 [polyamide]	17—22	17—18	19—23
Polystyrene	17—22	19	—
Poly(vinyl acetate)	17—19	—	—
Poly(vinyl chloride)	17—23	16—22	—
Phenolic resins	17—24	16—27	19—28
Buna N (butadiene-acrylonitrile copolymer)	18—19	—	—
Poly(methyl methacrylate)	18—26	17—27	—
Carbowax® 4000 [poly(ethylene oxide)]	18—26	17—30	19—30
Thiokol® [poly(ethylene sulfide)]	18—21	—	—
Polycarbonate	19—22	19—21	—
Pliolite® P-1230	19—22	—	—
Mylar® [poly(ethylene terephthalate)]	19—22	19—20	—
Vinyl chloride-acetate copolymer	19—23	16—27	—
Polyurethane	20—21	—	—
Styrene-acrylonitrile copolymer	22—23	19—20	—
Vinsol® [rosin derivative]	22—24	16—27	19—26
Epon® 1001 [epoxy]	22—24	17—27	—
Shellac	—	21—23	19—29
Polymethacrylonitrile	—	22—23	—
→ Cellulose acetate	23—26	21—30	—
Cellulose nitrate	23—26	16—30	26—30
Polyacrylonitrile	—	25—29	—
Poly(vinyl alcohol)	—	—	25—27
Nylon 6.6 [poly(hexamethylene adipamide)]	—	—	28—31
→ Cellulose	—	—	30—33

FORMELLA, BRAUMANN, ELMHORST (MARTIN BRINKMANN)
TCRC, WINSTON SALEM, NC 1990

SMOKE SEMIVOLATILES OF CIGARETTES WITH CA- AND PP-FILTERS (high pressure drop)



MULTIPLE OF SEMIVOLATIVE CHEMICAL IN PP FILTERED SMOKE VS CA FILTERED SMOKE

AVG = 2.1X

RANGE = 1.4X - 4.0X

2023952010

SUMMARY

EXPECTED INTERACTIONS OF CHEMICALS AND POLYMERS

- SOME POLYMERS WILL ABSORB A RANGE OF δs OF CHEMICALS.

- SOME POLYMERS WILL ABSORB MULTIPLE RANGES OF δs OF CHEMICALS.

- DESIGNED POLYMERS MIGHT ABSORB TARGETED CHEMICALS.

- COPOLYMERS AND POLYMER BLENDS MIGHT OFFER WIDE RANGING ALTHOUGH TARGETABLE CHEMICAL ABSORPTION CHARACTERISTICS.

- THERMODYNAMICS INDICATE THE ABOVE AS GENERALITIES BUT THEORIES ARE INSUFFICIENT TO PREDICT INTERACTIONS BETWEEN SPECIFIC POLYMERS AND CHEMICALS. (MOLECULAR MODELING MAY OFFER ADDITIONAL HELP.)

- KINETICS COULD BE A WILD CARD.

$\delta \equiv$ SOLUBILITY PARAMETER

OBJECTIVE

IDENTIFY AND DEVELOP POLYMERS

FOR SELECTIVE FILTRATION APPLICATIONS

PROBABLY LEADING TO,

BUT NOT LIMITED TO:

A MELT SPUN HETEROFIL

HAVING
A CORE POLYMER
WITH ROBUST FIBER PROPERTIES

AND
A SHEATH POLYMER
HAVING SELECTIVE FILTERING PROPERTIES.

PRODUCT DEVELOPMENT STRATEGY

SELECTIVE FILTERING POLYMERS FOR TOBACCO SMOKE

♦ DEVELOP POLYMER SCREENING TECHNIQUES THAT SIMULATE SMOKE/FILTER INTERACTIONS IN CIGARETTES.

♦ SCREEN A NUMBER OF AVAILABLE POLYMERS.

♦ VERIFY RESULTS WITH STANDARD TESTS ASAP.
- LAB-PREPARE PROTOTYPE FIBERS (FEW LBS).
- HAND PACK FILTERS & STD TOBACCO COLUMNS.
  * WHOLE SMOKE ANALYSIS.
  * VOLUNTEERS TASTE 'FILTERED' SMOKE.

♦ IDENTIFY A SECOND ROUND OF POLYMERS, COPOLYMERS OR BLENDS -- ANTICIPATING INSIGHTS!! UNIQUE MATERIALS?

♦ CHARACTERIZE PROPERTIES OF SECOND ROUND MATERIALS.

♦ VERIFY RESULTS (AS ABOVE).

♦ DEVELOP PILOT QUANTITIES OF CANDIDATE MATERIALS.

♦ CONDUCT PRODUCT AND MARKET ASSESSMENTS.

♦ CHOOSE TO DEVELOP PRODUCT AND MARKETS ....OR NOT.

2023957013

SCREENING POLYMERS FOR TOBACCO SMOKE SELECTIVE FILTRATION

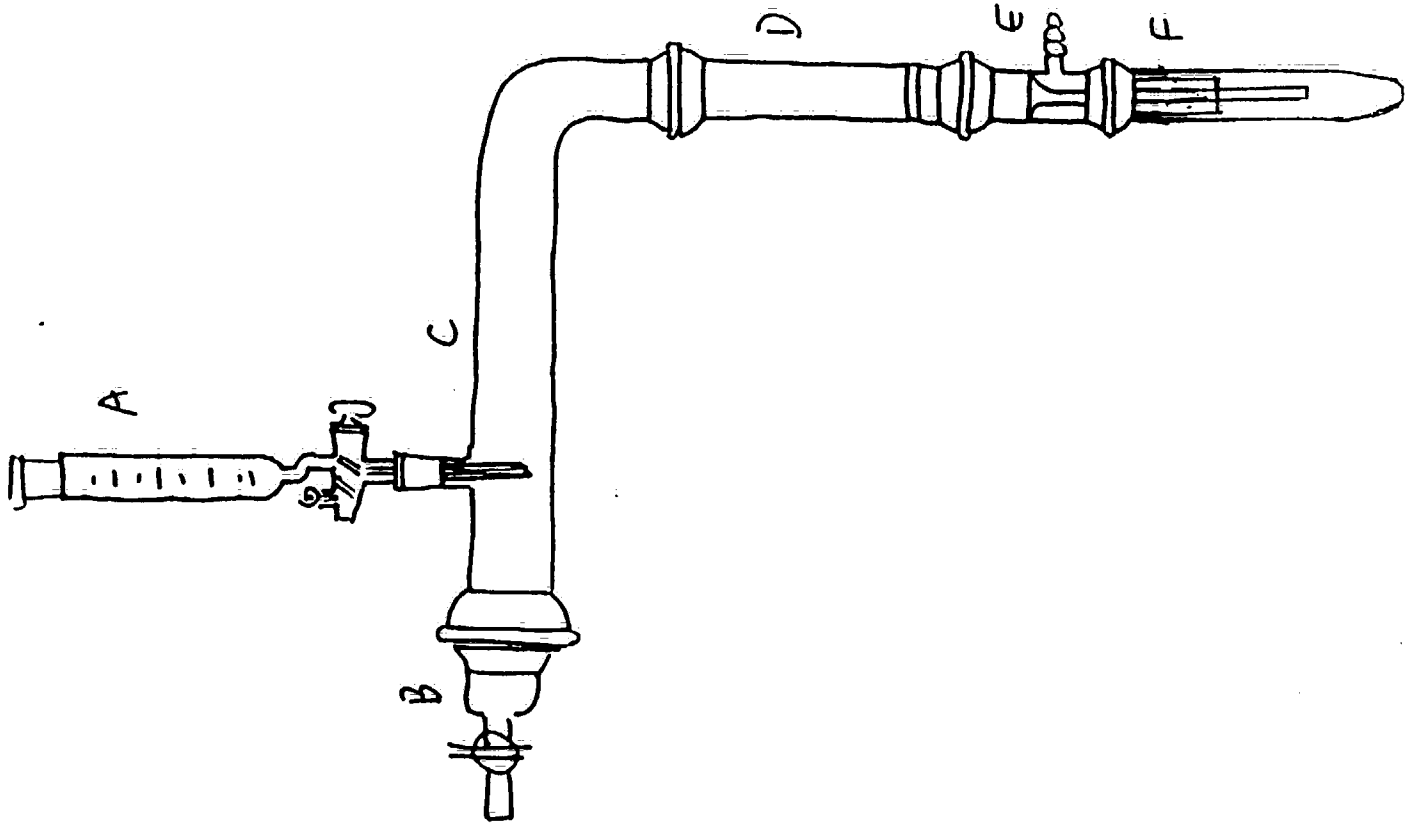
CONCEPT -- CONTROLLED SIMULATION OF SMOKE IN A FILTER

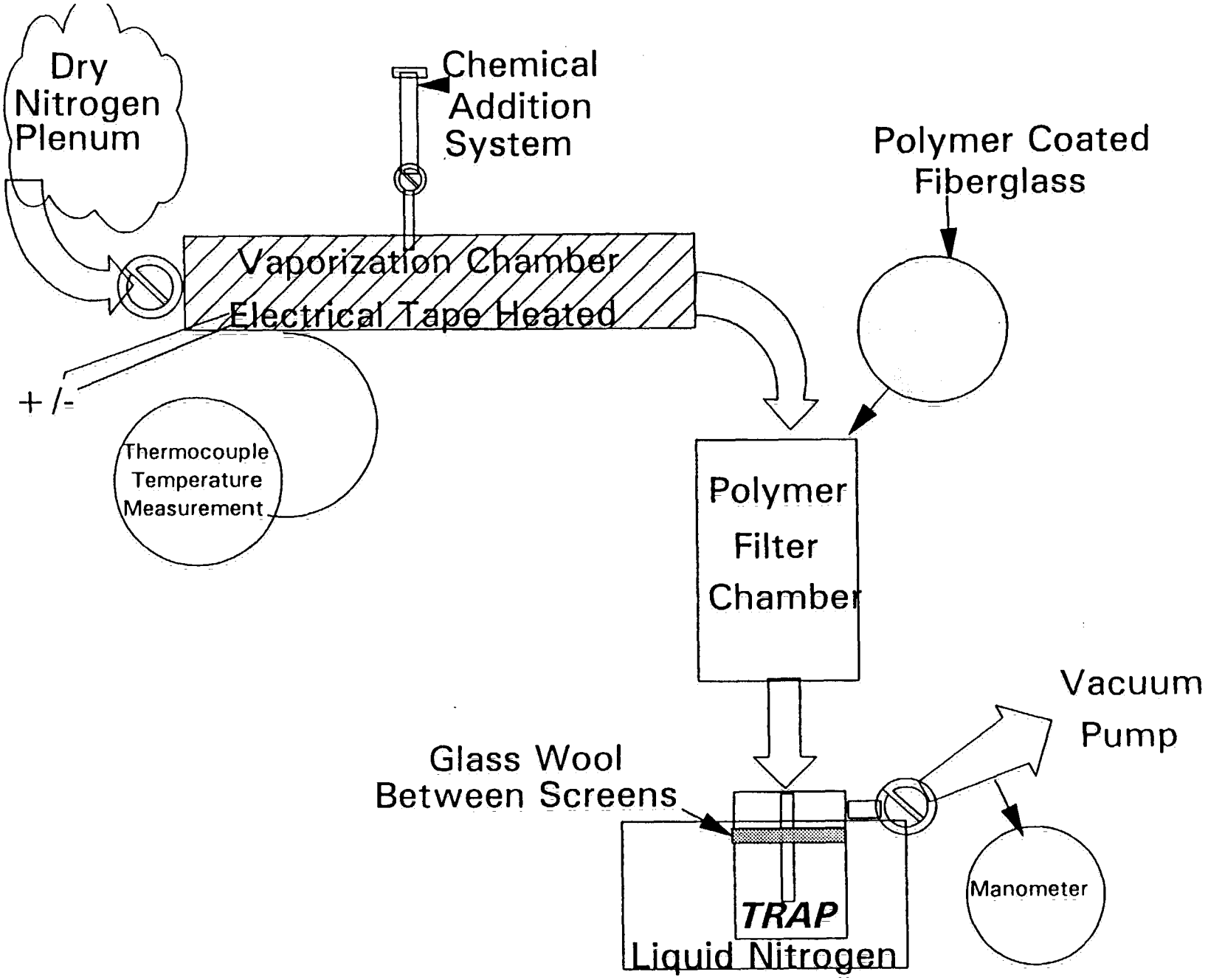
- ♦ FOCUS ON VOLATILE & SEMIVOLATILE CHEMICALS.
- ♦ SWEEP CHEMICALS OVER POLYMER (BRIEF EXPOSURE).
- ♦ COLLECT AND ANALYZE NON-ABSORBED CHEMICALS.
- ♦ CALCULATE CHEMICALS ABSORBED BY POLYMERS.
- ♦ USE CELLULOSE ACETATE AS A BENCH MARK.

SOME CONTROL ELEMENTS

- ♦ USE A SYNTHETIC SMOKE
  - LESS COMPLEX.
  - MORE REPRODUCIBLE.
- ♦ COAT POLYMERS ON ONE SUBSTRATE.
  - EQUALIZE FORM OF MANY POLYMERS.
- ♦ DEVELOP PROCEDURES FOR REPRODUCIBILITY.
- ♦ DEMONSTRATE REPRODUCIBILITY ASAP.

2023950014





MODIFIED TEST PROCEDURES

- ♦ HEAT CHAMBER #1 TO 200°C AND ELBOW TO 150°C.
- ♦ ADD SCREENS AND GLASS WOOL TO THE CONDENSER.
- Δ SWEEP HEATED APPARATUS WITH DRY NITROGEN.
- ♦ WEIGH ~1 G CHEMICALS IN A TARED ADDITION FUNNEL.
- ♦ ADD LIQUID N_2 TO TRAP.
- ♦ POLYMER/CHEMICAL INTERACTION:

  * PULL VACUUM FOR 10 SECONDS.
  * ADD ~ 0.05 GRAMS OF CHEMICALS TO CHAMBER.
  * USE N_2 TO EXPRESS CHEMICALS TO HEATED CHAMBER.
  * IMMEDIATELY, OPEN MAIN LINE TO N_2 PLENUM.
  * ALLOW N_2 TO SWEEP FOR 6 SECONDS.
  * CLOSE VACUUM AND N_2 LINES IN THAT ORDER.
  * ALLOW 2 MINUTES FOR THERMAL RE-EQUILIBRIUM.
  * REPEAT ABOVE STEPS.
  * AT END, ALLOW N_2 TO SWEEP THROUGH THE ADDITION FUNNEL AND CONDUCT 5 ADDITIONAL N_2 SWEEPS.

- ♦ REMOVE, SEAL, WARM, DRY AND WEIGH CONDENSATE RECEIVER.
- ♦ WASH FILTER AND RECEIVER WITH EG AND REWEIGH.
- ♦ GAS CHROMATOGRAPH THE CONDENSATE.

  - FID FOR ORGANIC COMPONENTS.

DATA HANDLING STRATEGY

$$\frac{W_i}{W_{EG}} = C_M \times \frac{GC_i}{GC_{EG}} + C_b$$

W_i = Weight of one component of mixture.

W_{EG} = Weight of ethyleneglycol

C_M = Measured Constant (slope)

GC_i = GC area for one component of mixture.

GC_{EG} = GC area for ethyleneglycol

C_b = Measured constant (intercept)

Weights of a given components --> multiply equation by W_{EG}

Normalized weight of component --> divide equation by a starting weight

To determine C_M and C_b, 35 similar chemical mixtures of known composition were diluted between 1:2 and 1:80 in ethyleneglycol, GC analyzed and submitted to regression analysis.

2025952018

ABOUT THE CHEMICALS

IN ORDER OF INCREASING GC RETENTION TIME	MG CHEMICAL IN 1 GRAM OF MIXTURE	R SQUARED IN REGRESSION ANALYSIS
ACETALDEHYDE	226	0.9820
FURAN	15	0.9254
ACETONE	96	0.9809
ACROLEIN	20	0.9624
METHANOL	19	0.9861
BENZENE	13	0.9716
2-PENTANONE	19	0.9732
ACETONITRILE	19	0.9875
TOLUENE	13	0.9394
PYRIDINE	25	0.9615
ACETIC ACID	219	0.9913
BENZOFURAN	40	0.9639
NICOTINE	173	0.9880
PHENOL	30	0.9901
GLYCEROL	36	0.9826

NEW Mixture D – Smoke Chemicals

Composition from Weights of Components used to Prepare Mixture

File Name _____ NB# _____ Dated _____

MIXTURE A	Approx. Wt. in Gms.	Approx. % of Total w/o Water	Actual Wt. in Gms.	% of Total From Wgts. w/o water	Organics Decimal Fraction
Water	36.0			----	----
Methanol	4.5	5.36		ERR	ERR
2–Pentanone	1.2	1.43		ERR	ERR
Acetone	8.2	9.76		ERR	ERR
Furan	1.2	1.43		ERR	ERR
Acrolein	1.7	2.02		ERR	ERR
Acetaldehyde	19.2	22.86		ERR	ERR
Total	72.0		0.0000		
Less Water	36.0		0.0000		
MIXTURE B					
Benzofuran	3.4	4.05		ERR	ERR
Acetonitrile	1.6	1.90		ERR	ERR
Pyridine	2.1	2.50		ERR	ERR
Nicotine	14.6	17.38		ERR	ERR
Benzene	1	1.19		ERR	ERR
Toluene	1.3	1.55		ERR	ERR
Total	24.0		0.0000		
MIXTURE C					
Phenol	2.6	3.10		ERR	ERR
glycerol	3.0	3.57		ERR	ERR
Acetic Acid	18.4	21.90		ERR	ERR
Total	24.0		0.0000		
Total Pct(%)		100.00		ERR	
D MIXTURE					
Mixture A	9.0				
Mixture B	3.0				
Mixture C	3.0				
Total	15.0		0.0		
Total less Water	10.5		ERR		
Percent Water in D		30		ERR	

*****SELECTIVE FILTRATION WORK SHEET – ETHYLENE GLYCOL IS THE INTERNAL STANDARD*****

File Name	Wgt D Inj	Gms	Org. Injectd	0.0000	Gms
Run Date	Wgt of Condensate	Gms	Org. Cndsd	ERR	Gms
NB Ref No	Wgt of EG	Gms	Water Inj	0.0000	Gms
Date GC Analys			Org Lost	ERR	Gms
D Mixture ID	Pct H2O in D	%	vs Org Inj	ERR	%
Date D Mixed	Percent D Condensed	ERR %	vs D Injctd	ERR	%

Polymer Coating

Synthetic Smoke Components Collected

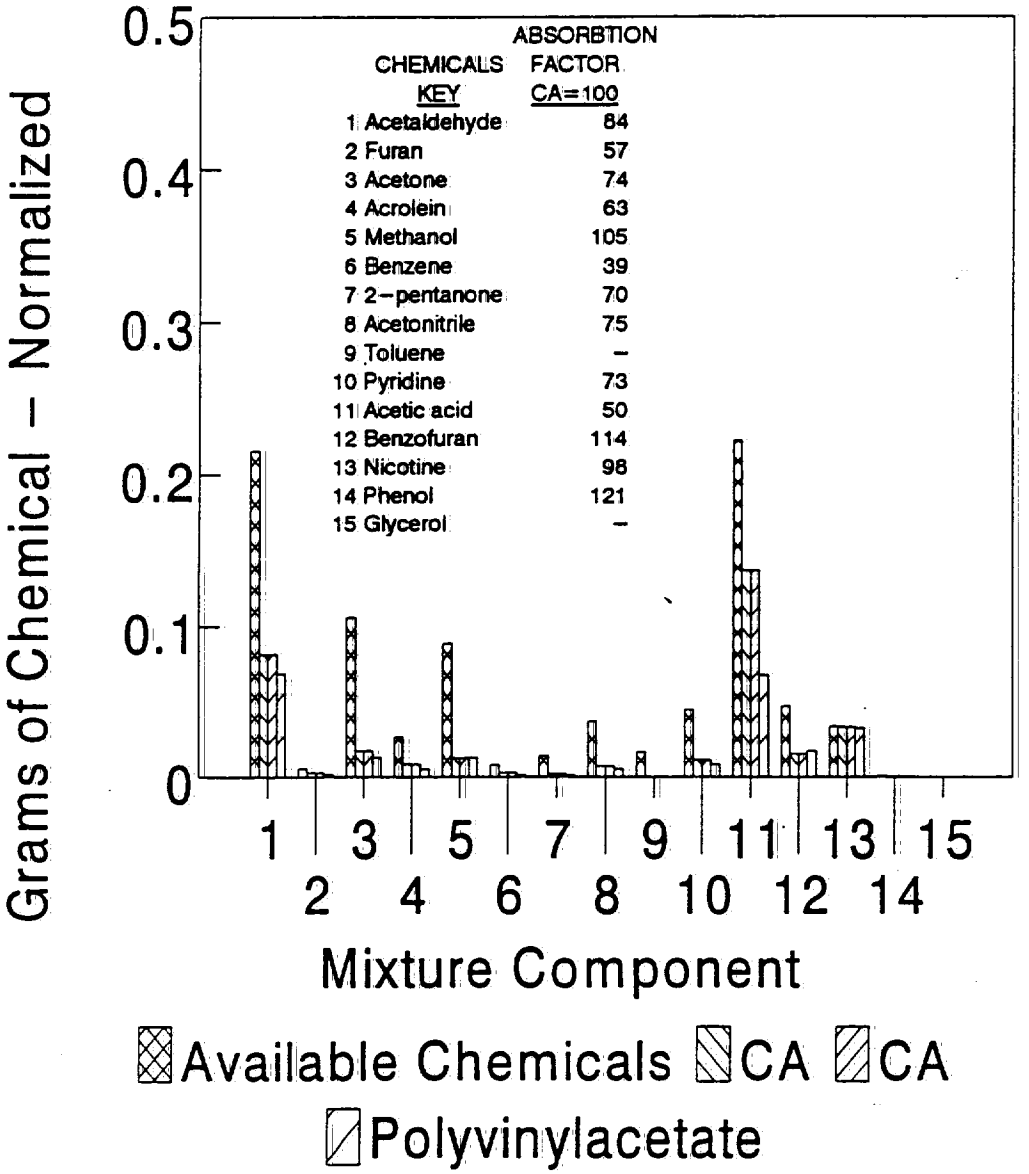
Chemical	Retention Time	Area 1	Area 2	GC Area Coefficient	Chem Wgt Constant	Wgt Condnsd per Gram of Organics Injctd
Acetaldehyde				1.1517	0.0014	ERR
Furan				0.6836	0.0002	ERR
Acetone				0.6836	0.0004	ERR
Acrolein				0.7131	0.0003	ERR
Methanol				0.9486	0.0001	ERR
Benzene				0.3683	0.0000	ERR
2–pentanone				0.5108	0.0001	ERR
Acetonitrile				0.6806	0.0000	ERR
Toluene				0.3407	0.0001	ERR
Pyridine				0.3830	0.0000	ERR
Acetic acid				1.3960	0.0009	ERR
Benzofuran				0.4250	0.0002	ERR
Nicotine				0.3746	0.0002	ERR
Phenol				0.3854	0.0000	ERR
Glycerol				0.9335	0.0000	ERR
EG					Total	ERR
Total Area	----					
Total minus Assigned Areas		0	0	Unassigned Areas as Pct of		
Total Smoke Chemical Areas		0	0	Smoke Chemical Areas	ERR %	

Vacuum, Empty Tube	mm Hg			
Vacuum, Filled Tube	mm Hg			
Weight of Coated Fiber	Grams			
Percent Coating on Fiber	%	From	% Solution of polymr in	

COMMENTS:

DATA IS NORMALIZED AGAINST THE WEIGHT OF THE ORGANIC COMPONENTS INJECTED

Chem. Absorb. by Polyvinylacetate Versus CA Absorption

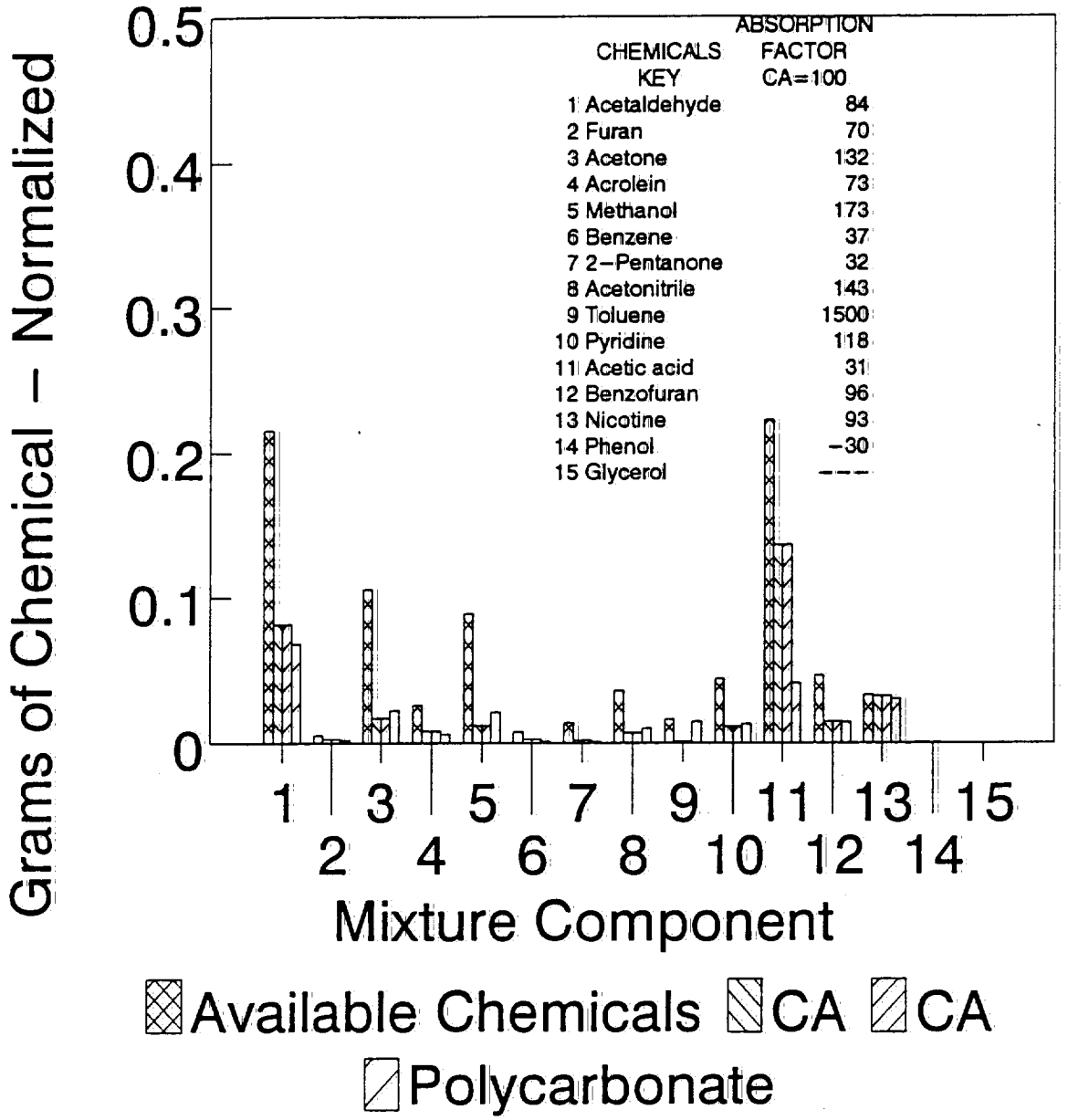


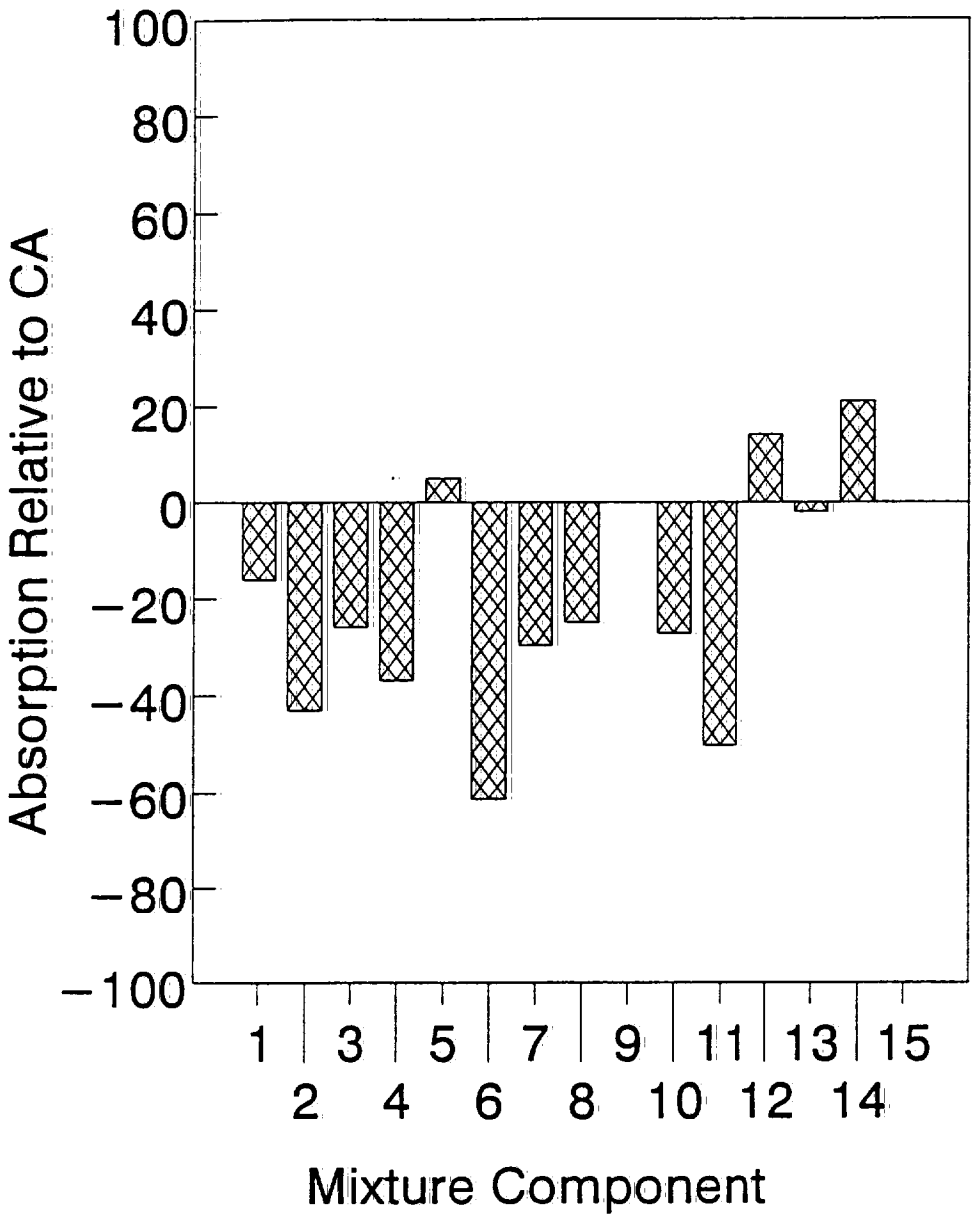
2023570222

Hoechst Celanese

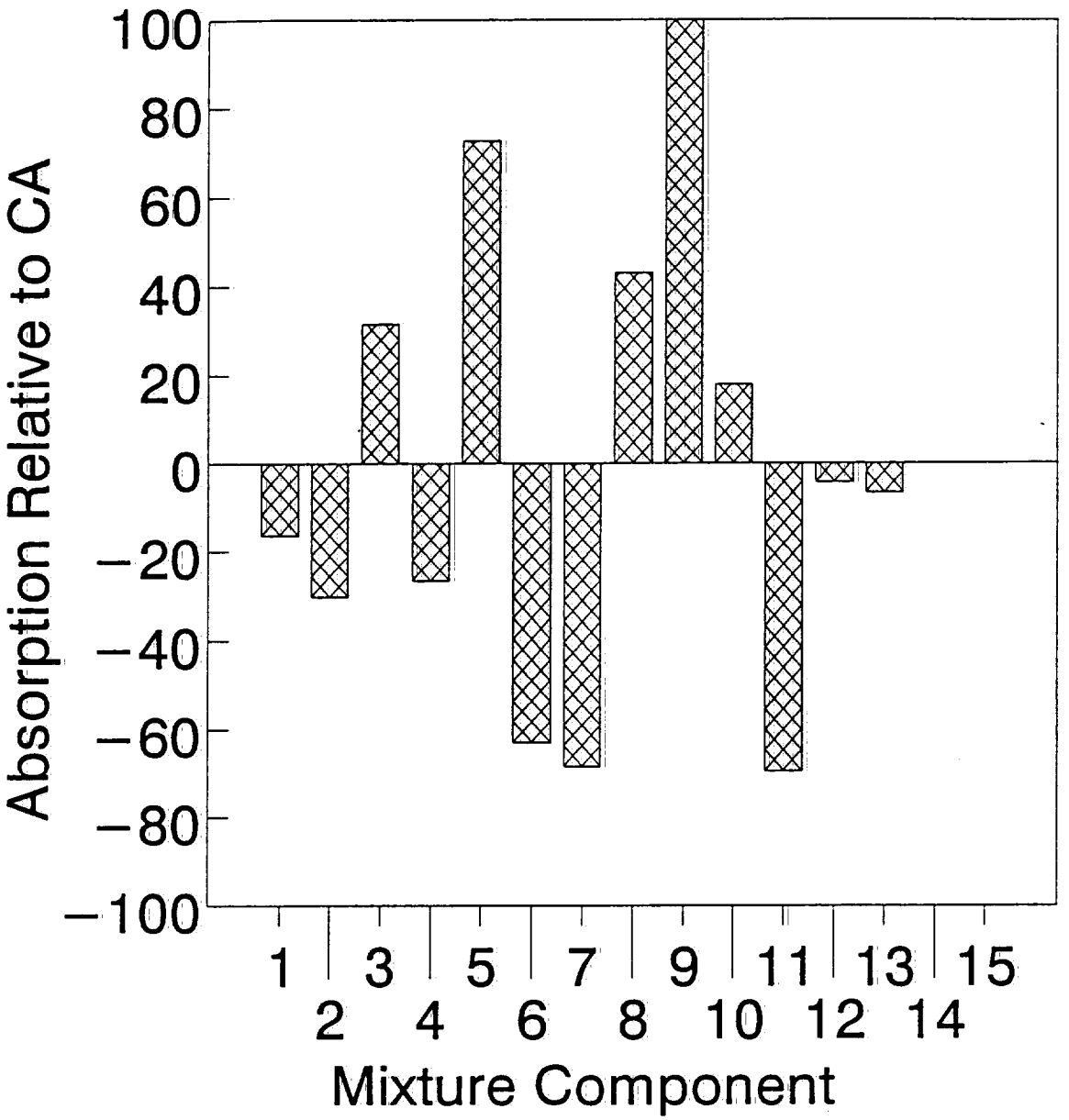
Hoechst

Chem. Absorb. by Polystyrene Versus CA Absorbtion

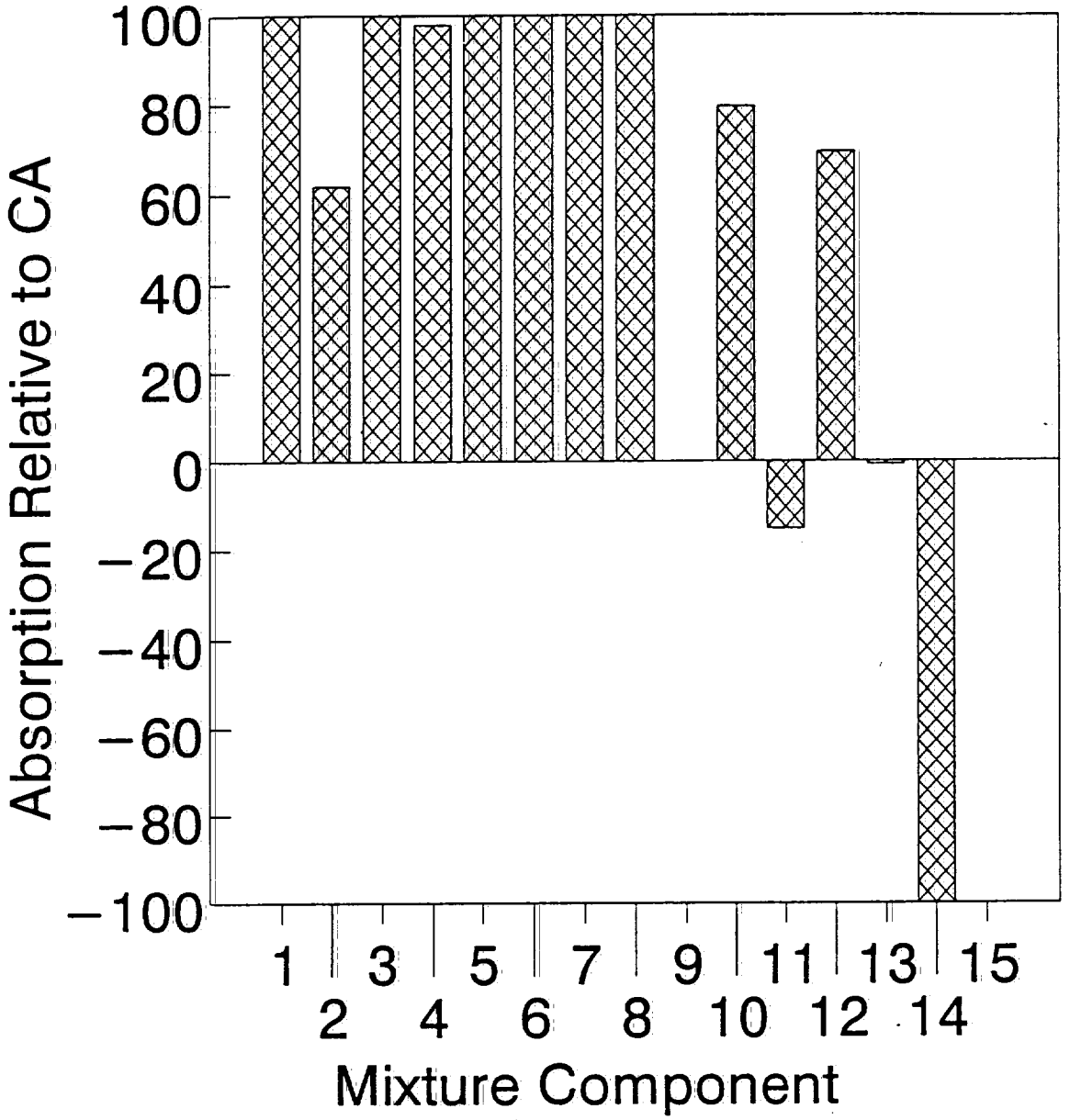




Relative Absorb. by Polystyrene Compared to CA (CA=0)



Relative Absorb. by Microcrystaline WAX Compared to CA (CA=0)



CAUTION: More water condensed than was injected.

STATUS OF PROGRAM

December 1993

- ADDRESSING HYPOTHESIS OF VARIABLE GLASS SURFACE-SORPTION IN BLANK RUNS FAILED TO IMPROVE PRECISION.

- ADDRESSING ALTERNATE HYPOTHESES FINALLY DEMONSTRATED PRECISION
  - ONE HYPOTHESIS TESTED AT A TIME
    - REDESIGNED SEVERAL APPARATUS PARTS
    - MODIFIED PROCEDURES
  - SIGNIFICANTLY IMPROVED STATISTICS
    - STD DEV FELL FROM .24 TO .04 ON AVGS OF ~0.5

- SPECIFIC CORRELATION COEFFICIENTS AND CONSTANTS WERE DEVELOPED FOR THE OUR COMBINATION OF CHEMICALS AND INTERNAL STANDARD (EG)

- ADSORPTION OF CHEMICALS BY CA FOUND TO BE LOW
  - CA IS A STRONG ABSORBER
  - WEAKER BUT SPECIFIC ABSORBERS MIGHT BE MISSED

COMPILED DATA FOR BLANK AND CA RUNS INDICATED

File Name	3-292BL2	3-293BLK	3-300CA	3-301CA	3-302CA	3-295CA	3-305CA1	3-305CA2	3-306CA
Run Date	10-19-93	10-20-93	102-27-9	10-28-93	10-29-93	10-22-93	11-1-93	11-1-93	11-2-93
Date GC Analys	10-21-93	10-27-93	10-28-93	10-28-93	11-4-93	10-27-93	11-3-93	11-3-93	11-3-93
D Mixture ID	10-19-93	10-19-93	10-19-93	10-19-93	10-19-93	10-19-93	10-19-93	10-19-93	10-19-93
Polymer Coating	None	None	10% CA	10% CA	10% CA	5% CA	5% CA	5% CA	5% CA
Wgt D Inj	1.11	1.024	1.147	1.121	1.118	1.121	1.137	1.127	1.114
Condensate	0.781	0.714	0.789	0.822	0.733	0.994	0.885	0.668	0.703
Wgt of EG	10.375	9.875	10.7	10.077	9.282	11.362	10.529	10.331	10.023
Pct H2O in D	29.88	29.88	29.88	29.88	29.88	29.88	29.88	29.88	29.88
Percent D Condensed	70.36	69.73	68.79	73.33	65.56	88.67	77.84	59.27	63.11
Org. Injectd G	0.7783	0.7180	0.8043	0.7860	0.7839	0.7860	0.7973	0.7903	0.7811
Org. Cndsd G	0.4745	0.4563	0.4257	0.3827	0.4074	0.3502	0.3744	0.3627	0.4550
Water Inj G	0.3317	0.3060	0.3427	0.3350	0.3341	0.3350	0.3397	0.3367	0.3329
Org Lost G	0.3038	0.2618	0.3785	0.4034	0.3765	0.4359	0.4228	0.4276	0.3261
vs Org Inj %	39.04	36.46	47.07	51.32	48.03	55.45	53.03	54.11	41.75
vs D Injctd %	27.37	25.56	33.00	35.98	33.68	38.88	37.19	37.94	29.27
	GRAMS OF COMPONENT CONDENSED /GRAM OF ORGANICS INJECTED					GRAMS OF COMPONENT CONDENSED /GRAM OF ORGANICS INJECTED			
Chemical									
Acetaldehyde	0.177	0.211	0.155	0.151	0.152	0.161	0.147	0.149	0.163
Furan	0.015	0.017	0.014	0.014	0.012	0.018	0.014	0.015	0.017
Acetone	0.079	0.088	0.078	0.076	0.077	0.073	0.074	0.076	0.083
Acrolein	0.017	0.019	0.015	0.015	0.014	0.014	0.014	0.014	0.015
Methanol	0.042	0.046	0.040	0.039	0.043	0.032	0.037	0.036	0.042
Benzene	0.010	0.010	0.008	0.009	0.008	0.009	0.008	0.008	0.009
2-pentanone	0.012	0.012	0.012	0.012	0.012	0.010	0.010	0.010	0.012
Acetonitrile	0.016	0.017	0.014	0.014	0.013	0.012	0.013	0.013	0.015
Toluene	0.013	0.013	0.013	0.014	0.013	0.012	0.013	0.012	0.014
Pyridine	0.019	0.021	0.018	0.017	0.021	0.012	0.016	0.015	0.019
Acetic acid	0.134	0.132	0.107	0.087	0.100	0.060	0.088	0.071	0.124
Benzofuran	0.032	0.034	0.029	0.030	0.029	0.020	0.025	0.022	0.033
Nicotine	0.042	0.015	0.027	0.010	0.026	0.011	0.011	0.017	0.034
Phenol	0.003	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.003
Glycerol	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Total	0.610	0.635	0.529	0.487	0.520	0.445	0.470	0.459	0.583
Unnacounted Condensed Wgt.	-0.025	-0.048	0.021	0.104	-0.009	0.309	0.171	-0.031	-0.085
Vac Empty tube	2.5	2.5	2.5	2.6	2.6	2.5	2.5	2.7	2.9
Vacuum filled	2.9	3	2.8	2.9	2.9	2.9	2.8	3	3.3
Drop with Fiber	0.4	0.5	0.3	0.3	0.3	0.4	0.3	0.3	0.4
Wgt Coated Fiber	41.95	38.38	31.35	20.63	24.54	38.97	33.58	37.29	34.64
Percent Coating	None	None	12.24	12.24	12.24	5.27	5.27	5.27	5.27

NOTE: Second group of experiment is the new lab. EG added to the cold trap at end of the run.

DATA IS NORMALIZED AGAINST THE WEIGHT OF THE ORGANIC COMPONENTS INJECTED

Chemicals Injected and Condensed after Exposure to a Blank or CA

Chemical	G of Chem in 1 G of Org injctd	Avg 2 Runs G chem Thru blank	Range as Percent of Average	Avg 3 Runs G Cndsd w 10% CA	Range as Percent of Average	Avg 4 Runs G Cndsd w 5% CA	Range as Percent of Average
Acetaldehyde	0.225	0.194	17.5	0.153	2.6	0.155	10.7
Furan	0.019	0.016	14.4	0.013	12.9	0.016	26.5
Acetone	0.097	0.084	10.2	0.077	2.0	0.076	12.7
Acrolein	0.022	0.018	14.8	0.014	5.9	0.014	9.2
Methanol	0.055	0.044	7.3	0.041	8.9	0.037	26.3
Benzene	0.012	0.010	0.7	0.008	9.3	0.009	20.4
2-pentanone	0.014	0.012	3.7	0.012	3.2	0.011	19.2
Acetonitrile	0.019	0.016	8.1	0.014	5.8	0.013	26.5
Toluene	0.017	0.013	0.3	0.013	9.0	0.013	17.5
Pyridine	0.025	0.020	9.9	0.019	21.9	0.016	46.1
Acetic acid	0.221	0.133	1.2	0.098	20.2	0.086	74.0
Benzofuran	0.040	0.033	6.7	0.029	3.2	0.025	49.8
Nicotine	0.172	0.028	95.5	0.021	83.7	0.018	128.3
Phenol	0.032	0.002	109.3	0.001	64.9	0.001	164.5
Glycerol	0.032	0.000		0.000		0.000	
Total	1	0.623		0.512		0.489	
Average			4.1		8.3		28.0

NOTE: Second group of experiment is the new lab. EG added to the cold trap at end of the run.

2023957029

CHEMICALS AVAILABLE AND ABSORBED BY CA

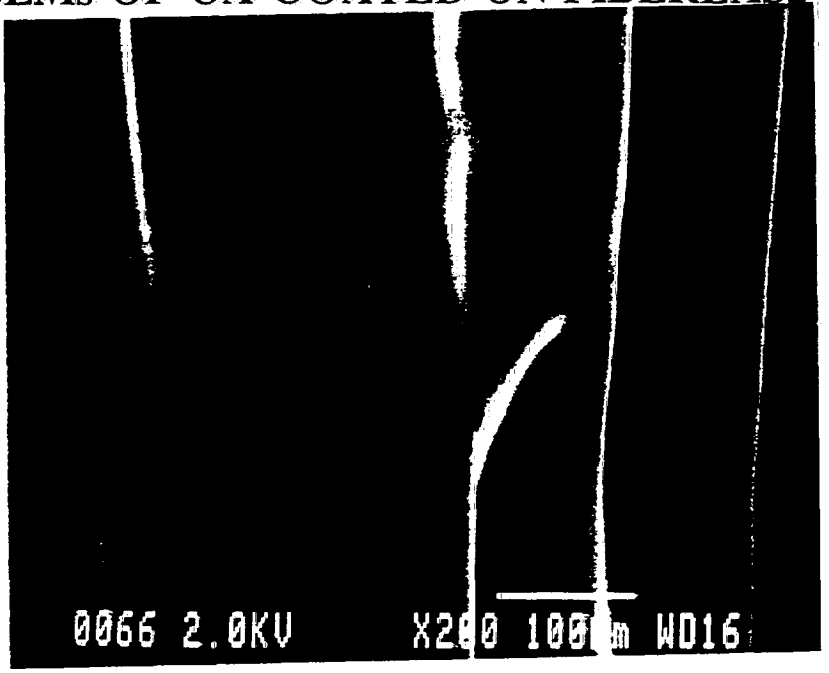
From 10/19/93 thru 11/2/93 Runs

Chemical	Grams of Chemical /G Org Inj	Avg 2 Runs Condensat Thru Blank	Range of Blank Data	Avg 3 Runs Absorption by 10% CA	Range of 10% CA Data	Avg 4 Runs Absorption by 5% CA	Range of 5% CA Data
Acetaldehyde	0.225	0.194	0.034	0.041	0.002	0.039	0.017
Furan	0.019	0.016	0.002	0.003	0.001	0.001	0.004
Acetone	0.097	0.084	0.009	0.007	0.001	0.007	0.010
Acrolein	0.022	0.018	0.003	0.004	0.000	0.004	0.001
Methanol	0.055	0.044	0.003	0.003	0.002	0.007	0.010
Benzene	0.012	0.010	0.000	0.001	0.000	0.001	0.002
2-pentanone	0.014	0.012	0.000	0.001	0.000	0.002	0.002
Acetonitrile	0.019	0.016	0.001	0.003	0.000	0.003	0.004
Toluene	0.017	0.013	0.000	0.000	0.001	0.000	0.002
Pyridine	0.025	0.020	0.002	0.001	0.002	0.004	0.007
Acetic acid	0.221	0.133	0.002	0.035	0.010	0.047	0.064
Benzofuran	0.040	0.033	0.002	0.004	0.000	0.008	0.013
Nicotine	0.172	0.028	0.027	0.007	0.009	0.010	0.023
Phenol	0.032	0.002	0.002	0.001	0.000	0.001	0.002
Glycerol	0.032	0.000	0.000	0.000		0.000	0.000
Total	1	0.623		0.111		0.133	

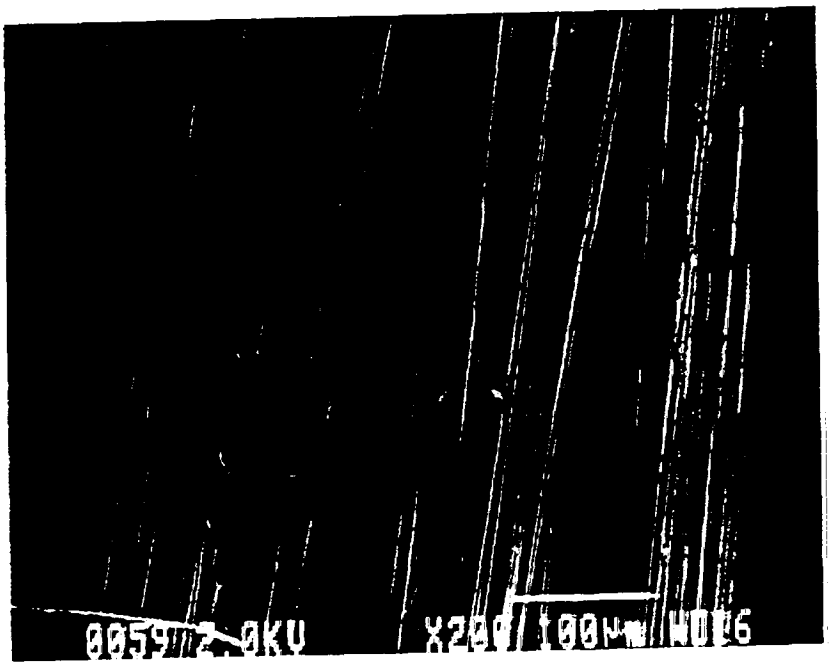
PROSPECTS FOR INCREASING CHEMICAL SORPTION BY POLYMERS IN THE SELECTIVE FILTRATION TEST

- EXCELLENT
  - ▲ UP TO NOW, > 1000 FIBERGLASS FILAMENTS HAVE BEEN ENCAPSULATED IN POLYMER FOR USE IN THE TEST.
    - ▼ PRELIMINARY DATA HAD INDICTED THAT SORPTION WOULD BE ENOUGH.
  - ▲ POLYMER SURFACE AREA CAN BE INCREASED BY ORDERS OF MAGNITUDE BY COATING FILAMENTS
- TOW BANDING DEVICES WILL BE EVALUATED
- OTHER TECHNOLOGY CAN BE TAPPED IF NEEDED

SEMs OF CA COATED ON FIBERLASS



10% CA on DE37 Fiberglass



5% CA on DE37 Fiberglass

REVISED MILESTONES

1/94 IDENTIFY A FIBERGLASS THAT WILL OPEN WELL FOR COATING FILAMENTS.

2/94 DEVELOP CONDITIONS FOR REPRODUCIBLE COATING OF FIBERGLASS FILAMENTS.

3/94 ESTABLISH BASE DATA FOR THE NEW BLANK AND CA COATED FIBER IN THE TEST.

6/94 CHARACTERIZE SELECTIVE ABSORPTION CHARACTERISTICS OF A DOZEN OR MORE COMMERCIAL POLYMERS.

include PP+polyp filters (Rayon)

7/94 EVALUATE PROGRAM. SELECT CANDIDATES.

9/94 PREPARE LABORATORY QUANTITIES OF FIBER(S) FROM 'INTERESTING' SELECTIVE FILTERING POLYMERS FOR STANDARD TESTING IN HAND-ASSEMBLED CIGARETTES.

9/94 ACQUIRE ADDITIONAL POLYMERS, COPOLYMERS AND BLENDS FOR SECOND ROUND OF LAB-TEST CHARACTERIZATIONS.

10/94 RUN STANDARD SMOKE CHEMISTRY TESTS ON HAND PACKED CIGARETTES WITH LAB-MADE FIBER IN FILTERS. VOLUNTEERS INDICATE TASTE KNOCK-OUTS (HARSH, BITTER ETC).

12/94 CHARACTERIZE SECOND ROUND OF SELECTIVE ABSORBING MATERIALS

1/95 RECOMMEND PLANS FOR CONTINUING RESEARCH, STARTING DEVELOPMENT OR NOT.

2023957033